

Isobutylmalonic acid
4361-06-2 | DTXSID60195885

Model Performance

| | |
|-------|------|
| Model | Data |
|-------|------|

Weighted KNN model

| 5-fold CV (75%) | | Training (75%) | | Test (25%) | |
|-----------------|------|----------------|------|------------|------|
| Q2 | RMSE | R2 | RMSE | R2 | RMSE |
| 0.72 | 51.8 | 0.74 | 50.3 | 0.73 | 52.7 |

Model Results

Predicted value: 96.2 °C

Global applicability domain: Inside

Local applicability domain index: 8.41e-01

Confidence level: 6.42e-01

Nearest Neighbors from the Training Set

| | | |
|----------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------|
| <div>Image not found</div> <div>Pentanedioic acid, 3,3-dimethyl-</div> <div>Measured: 104</div> <div>Predicted: 96.7</div> | <div>Image not found</div> <div>2-METHYLHEXANEDIOIC ACID</div> <div>Measured: 64.0</div> <div>Predicted: 90.6</div> | <div>Image not found</div> <div>2,2-Dimethylpentanedioic acid</div> <div>Measured: 84.0</div> <div>Predicted: 90.5</div> |
| <div>Image not found</div> <div>Octanedioic acid</div> <div>Measured: 144</div> <div>Predicted: 115</div> | <div>Image not found</div> <div>3-Ethyl-3-methylglutaric acid</div> <div>Measured: 87.0</div> <div>Predicted: 88.7</div> | |